

Chemistry 430 — Simulation in Chemistry & Biochemistry

Laboratory Report Format:

In order to complete each lab project, you should write a short "report" with the sections outlined below. These should be turned in to Jay Ponder (email or in person), preferably within about two weeks following the date of the lab period.

- (1) Introduction** -- brief summary of the objectives for the project; typically does not need to be more than a couple of sentences
- (2) Procedure** -- what steps did you actually perform, and in what order; do not repeat what is in the lab protocol, you only need to describe things you have done that are not in the original supplied procedure
- (3) Methods** -- kinds of calculations, programs used, level of theory, assumptions or approximations such as quantities varied, restraints or constraints, special program options, *etc.*; do not repeat the supplied protocol
- (4) Results** -- data obtained, usually presented as both tables and plots; this is generally the major section of the report
- (5) Analysis** -- explain your results; why did things turn out as they did, what can you find in texts or published papers to support your interpretation of the data (*i.e.*, for this specific system or for analogous systems)
- (6) Conclusions** -- what lessons were learned from this project, what kinds additional calculations could be done to further explore the topic; this section can be very brief and just summarize main points
- (7) Questions** -- answer specific questions provided as part of the project, including results and analysis from any additional calculations you performed

Again, sections (1), (2), (3) and (6) can be short. Sections (4), (5) and (7) will be the key parts of a report. It is not necessary to include a lot of extra prose. The point of the report is to document that you completed the lab, were able to analyze and make sense of the results, and discuss related topics as in the included questions.